

A marginal observer's effective thermodynamics

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Nonequilibrium thermodynamics often presumes that the observer has complete information about the system he/she deals with: no parasitic current, exact evaluation of the forces that drive the system. For example, the acclaimed Fluctuation Relation (FR), relating the probability of time-forward and time-reversed events, holds on the assumption that measurable transitions suffice to characterize the process as Markovian (in our case, a continuous-time “jump” process). However, most often the observer only measures *marginal* information. We show that he/she will nonetheless produce an *effective* description that does not dispense with the fundamentals of thermodynamics, including the FR and the 2nd Law. The results stand on the crucial notion of hidden time-reversal of the dynamics, considering one single transition in configuration space as the observational current. We use a simple example to illustrate our results and discuss the feasibility of further generalizations.

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Nonequilibrium thermodynamics is a discourse about currents J_α flowing across an open system and about their cost, viz. the forces or affinities F_α that need to be exerted to sustain such flows. Statistical Mechanics adds up one further level of complexity by making currents into random variables J_α^t whose joint probability $P(J_\alpha^t)$ is determined by the occurrence of an underlying Markovian trajectory t in configuration space. Be them electric currents and voltages, heat flows and temperature gradients, etc., thermodynamics establishes certain universal truths, among which, in a progression that covers the long time-arch 19th to 21st century: (*2nd Law*) the average rate at which entropy is delivered to the environment $\sum F_\alpha \langle J_\alpha^t \rangle$ is non-negative; (*FDR*) near equilibrium a perturbation of the currents leads to Dissipation, which is Related to the current's Fluctuations; (*FR*) the probability of observing positive Fluctuations of the entropy delivery rate is exponentially favoured if Related to negative (or time-reversed) ones [1]:

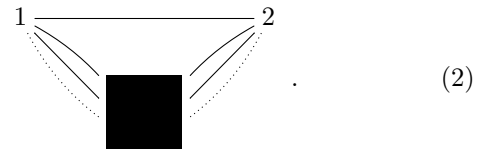
$$\frac{P(J_\alpha^t)}{P(-J_\alpha^t)} = \exp t \sum F_\alpha J_\alpha^t. \quad (1)$$

Notoriously, the FR holds in the long-time limit (but it can be formulated at all times [2–4]). To avoid certain routine complications with time scalings [5], we will choose rates fast enough as to make time $t \equiv 1$ sufficiently large so that the system is at steady-state.

The above results require that all possible sources of dissipation are known. However, most often such a complete description is impossible to achieve, neither experimentally (leakages of currents) nor theoretically (coarse-grained degrees of freedom [6, 7]). How can then thermodynamics be established in self-consistent way? In this paper we consider a *marginal* observer who only monitors transitions between two given configurations and controls a parameter that only affects the rates of those transitions — taking the configuration space to be a fi-

nite connected graph. We show that such observer would guess an *effective* affinity such that *i*) a *marginal* FR for the observational current holds (see also Refs. [8–11] for analogous attempts at a marginal FR), requiring a modified notion of “time reversal” that only inverts the hidden currents; *ii*) the effective affinity has a clear interpretation as the counteracting force needed to *stall* the current, i.e. to make it vanish; *iii*) the FDR at stalling derived in Ref. [12] follows as a consequence; *iv*) while the “hidden time-reversed” dynamics does not have a clear operational implementation, it is an interesting mathematical construct rich in properties. At a first reading, proofs of theorems can be safely skipped.

Story of a marginal observer. Consider a *gedanken*-observer who can play with a measurement apparatus that only resolves two configurations, $i = 1, 2$. The rest of the world is a black box:



Our observer controls the rate $w_{12}(x)$ at which, *given* that the apparatus recorded 2, the pointer moves to 1 right afterwards, and similarly for $w_{21}(x)$. The observer can also record *how often* state 2 occurs with respect to state 1. This piece of information, which is independent of whether transition 12 even occurs, is quantified by the ratio $p_1(x)/p_2(x)$, where $\vec{p}(x)$ is the probability of being anywhere in state-space, including those black-box-states $p_{\blacksquare}(x)$ whose population is unknown. Finally, the observer handles a knob x by which he tunes to-and-fro rates. We assume, crucially, that this knob has no effect on the black box, and that x is *thermodynamic* in the sense that it would be the free energy (up to a ground

value x^*) if only transitions among 1 and 2 could occur:

$$\frac{w_{12}(x)}{w_{21}(x)} = e^{x-x^*}. \quad (3)$$

If the observer's world was complete and only transitions among 1 and 2 were possible, then the system would relax to equilibrium $\vec{p} = \vec{p}^{\text{eq}}$, no net current would be measured along 12, and detailed balance would imply

$$\frac{p_1^{\text{eq}}(x)}{p_2^{\text{eq}}(x)} = \frac{w_{12}(x)}{w_{21}(x)}. \quad (4)$$

Instead, it occurs that our observer measures a different value of $p_1(x)/p_2(x)$, yielding an average current $\langle J \rangle(x) := w_{12}(x)p_2(x) - w_{21}(x)p_1(x)$. The observer must then formulate a minimal model that is compatible with his observations. The simplest possible setup is

$$\begin{array}{c} w(x) \\ \text{1} \quad \text{2} \\ \text{---} \\ \tilde{w} \end{array} \quad (5)$$

In this minimal model the black box is responsible of returning an event at sites 1 or 2 at some effective rates $\tilde{w}_{12}, \tilde{w}_{21}$; while this is not a viable approximation for the full black-box dynamics, and more advanced methods need to be employed based on projection techniques [13], it is enough to describe the average steady-state measurements of our observer.

Notice that the minimal model satisfies the global detailed balance condition obtained by lumping the transitions w and \tilde{w} :

$$\frac{w_{21}(x) + \tilde{w}_{21}}{w_{12}(x) + \tilde{w}_{12}} = \frac{p_2(x)}{p_1(x)}. \quad (6)$$

We will now compare this quantity with the truth-of-matter of the complete system. To illustrate our results, we will employ the following example:

$$\begin{array}{ccc} \begin{array}{cc} 1 & \text{---} & 2 \\ | & \diagdown & | \\ 4 & \text{---} & 3 \end{array} & , & \begin{array}{cc} 1 & \rightleftharpoons & 2 \\ \uparrow & \diagdown & \downarrow \\ 4 & \rightleftharpoons & 3 \end{array} \xrightarrow{\text{TR}} \begin{array}{cc} 1 & \rightleftharpoons & 2 \\ \downarrow & \diagdown & \uparrow \\ 4 & \rightleftharpoons & 3 \end{array} \end{array} \quad (7)$$

The first diagram depicts the topology, where the graph's *edges* connect *sites* (configurations). The second depicts a steady state, with currents obeying Kirchhoff's law of current conservation at the sites of the graph, and the third its time-reversed (for later use).

The full system is assumed to evolve by the Master Equation $d\vec{p}(t)/dt = \mathbb{W}\vec{p}(t)$, with generator $\mathbb{W}_{ij} := w_{ij} - w_i\delta_{i,j}$, where rates $w_{ji}, w_{ij} > 0$ are assumed to be positive along all edges of the graph, and $w_i := \sum_k w_{ki}$ are the exit rates [14]. The steady state \vec{p} is the unique

null vector of \mathbb{W} . Let $\mathbb{W}_{(j_1, \dots, j_n | i_1, \dots, i_m)}$ be the matrix obtained by removing rows j_1, \dots, j_n and columns i_1, \dots, i_m . **Theorem:** *The effective rates are given by*

$$\tilde{w}_{12} = \frac{\begin{array}{c} \uparrow \downarrow + \uparrow \diagdown + \downarrow \diagup \\ \uparrow \quad \uparrow + \quad \uparrow \quad \uparrow + \quad \downarrow \quad \downarrow + \quad \downarrow \end{array}}{\det \mathbb{W}_{(2|1)}} = \frac{\det \mathbb{W}_{(2|1)}^{\text{st}}}{\det \mathbb{W}_{(1,2|1,2)}} \quad (8)$$

and similarly for \tilde{w}_{12} . Diagrams illustrate the multiplication of rates along oriented arrows. Notice that, rightly, the effective rates do not depend on x . **Proof:** Expanding with Laplace's formula the determinant $0 = \det \mathbb{W} = \sum_j \mathbb{W}_{ij}(-1)^{i+j} \det \mathbb{W}_{(i|j)}$, one finds that the steady-state probability can be written in terms of the minors of the generator, $p_i \propto (-1)^{i+j} \det \mathbb{W}_{(j|i)}$ (independently of j). By the matrix-tree theorem in algebraic graph theory, minors can be given a graphical representation in terms of oriented rooted spanning trees. We obtain

$$\begin{aligned} \frac{p_1(x)}{p_2(x)} &= \frac{\det \mathbb{W}_{(2|1)}(x)}{\det \mathbb{W}_{(1|2)}(x)} \\ &= \frac{\begin{array}{c} \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow \\ \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow \end{array}}{\begin{array}{c} \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow \\ \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \uparrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow + \leftarrow \downarrow \end{array}} \end{aligned} \quad (9)$$

Notice that there are five trees that pass through edge 12 and three trees that do not. These contributions can be singled out using the *deletion-contraction* formula in graph theory [15], which algebraically reads

$$\det \mathbb{W}_{(2|1)}(x) = w_{12}(x) \det \mathbb{W}_{(1,2|1,2)} + \det \mathbb{W}_{(2|1)}^{\text{st}}, \quad (10)$$

where \mathbb{W}^{st} is the *stalling* generator obtained from \mathbb{W} by setting $w_{12} \equiv w_{21} \equiv 0$. We can now compare to Eq. (6). Since it must hold for all x , we conclude \square .

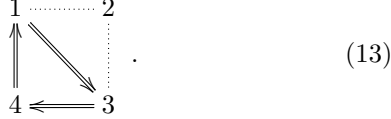
Effective affinity and stalling. Supporting a steady-state current has a thermodynamic cost. According to the theory of Hill-Schnakenberg [16, 17], this is given by cycle affinities, i.e. the log-ratio of products of rates along cycles, in the two directions. In the complete system, there are a number of "real" affinities $F_\alpha(x)$ depending on the number of cycles in the black box [24]. In the case of the minimal model, there only is one cycle, whose *effective affinity* is given by

$$\tilde{F}(x) = \log \frac{w_{12}(x)\tilde{w}_{21}}{w_{21}(x)\tilde{w}_{12}} = x - x^{\text{st}} \quad (11)$$

where we define the stalling value of the parameter as

$$x^{\text{st}} = x^* + \log \frac{\begin{array}{c} \downarrow \uparrow + \downarrow \uparrow + \downarrow \uparrow \\ \downarrow \uparrow + \downarrow \uparrow + \downarrow \uparrow \end{array}}{\begin{array}{c} \downarrow \uparrow + \downarrow \uparrow + \downarrow \uparrow \\ \downarrow \uparrow + \downarrow \uparrow + \downarrow \uparrow \end{array}} = x^* + \log \frac{p_1^{\text{st}}}{p_2^{\text{st}}}. \quad (12)$$

In this latter expression we recognized \vec{p}^{st} as the steady state of the stalling system where edge 12 is removed altogether, $\mathbb{W}^{\text{st}} \vec{p}^{\text{st}} = 0$. The effective affinity $\tilde{F} = \log \frac{w_{12} p_2^{\text{st}}}{w_{21} p_1^{\text{st}}}$ can then be interpreted as the force that needs to be exerted to sustain the current and avoid the system to fall in the stalling state. Such stalling state is reached when $x = x^{\text{st}}$, where the effective affinity and the marginal current vanish $\langle J^t \rangle(x^{\text{st}}) = 0$. Notice that, despite to the local observer the stalling state is a state of “marginal equilibrium”, yet in the black box arbitrary currents might be flowing [18], as for example in this configuration:



Fluctuations. So far we considered a minimal model reproducing the observer’s steady-state average measurements and predicting an effective thermodynamic cost of sustaining the observable current. The question we now address is: will this representation be consistent when it comes to fluctuations of the current?

Establishing the complete FR Eq. (1) requires a notion of time-reversed (TR) dynamics $\tilde{\mathbb{W}} := \mathbb{P} \mathbb{W}^T \mathbb{P}^{-1}$, where T denotes matrix transposition and $\mathbb{P} := \text{diag}\{p_i\}_i$ is the diagonal matrix whose diagonal entries are the steady-state probabilities. Denoting \bar{P} the probability associated to the TR dynamics, under time reversal currents change sign in probability $\bar{P}(J_\alpha) = P(-J_\alpha)$. In general the marginal probability for J^t will not satisfy a FR with respect to probability P . Yet, we will show that there exists a well-defined *hidden TR dynamics* such that the following *marginal FR* can be derived

$$\frac{P(J^t)}{\tilde{P}(-J^t)} = \exp \tilde{F} J^t, \quad (14)$$

where, quite remarkably, the effective affinity $\tilde{F} \equiv \tilde{F}(x)$ is precisely the one that our local observer estimates from his minimal model.

Before introducing the hidden TR dynamics, let us make a few observations and derivations. Importantly, but in the limit of a “fast box” [19], $P(J^t) \neq \tilde{P}(J^t)$, which leads to a substantial difference with respect to Eq. (1). While rates of the hidden TR dynamics are known, unless a clear *operational* definition is available it might be difficult to micro-engineer all rates and design experiments that test the marginal FR. However, integrating over J^t leads to the *marginal integral FR*

$$\left\langle \exp -\tilde{F}(x) J^t \right\rangle(x) = 1. \quad (15)$$

Notice that the average depends itself on x . Using Jensen’s inequality we can also obtain the effective second law $\tilde{F}(x) \langle J^t \rangle(x) \geq 0$ (see [6] for another perspective

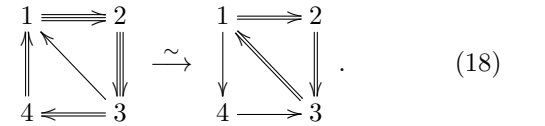
on coarse graining). Notice that the marginal integral FR only depends on the original dynamics, and not on the hidden TR dynamics, which is traced out (as in Ref. [20]). Hence it is experimentally accessible. Furthermore, by taking the second derivative with respect to x and evaluating at stalling we obtain the FDR [12]:

$$\frac{d}{dx} \langle J^t \rangle(x^{\text{st}}) = \frac{1}{2} \text{var}(J^t)(x^{\text{st}}). \quad (16)$$

Hidden TR dynamics. The generator of the hidden TR dynamics is defined as

$$\begin{aligned} \tilde{\mathbb{W}}(x) &:= \overbrace{\mathbb{W}(x) - \mathbb{W}_{\text{st}}}^{\text{12-block}} + \mathbb{P}_{\text{st}} \mathbb{W}_{\text{st}}^T \mathbb{P}_{\text{st}}^{-1} \\ &= \begin{pmatrix} -w_1(x) & w_{12}(x) & w_{31} \frac{p_1^{\text{st}}}{p_3^{\text{st}}} & w_{41} \frac{p_1^{\text{st}}}{p_4^{\text{st}}} \\ w_{21}(x) & -w_2(x) & w_{32} \frac{p_2^{\text{st}}}{p_3^{\text{st}}} & 0 \\ w_{13} \frac{p_3^{\text{st}}}{p_1^{\text{st}}} & w_{23} \frac{p_3^{\text{st}}}{p_2^{\text{st}}} & -w_3 & w_{43} \frac{p_3^{\text{st}}}{p_4^{\text{st}}} \\ w_{14} \frac{p_4^{\text{st}}}{p_1^{\text{st}}} & 0 & w_{34} \frac{p_4^{\text{st}}}{p_3^{\text{st}}} & -w_4 \end{pmatrix} \end{aligned} \quad (17)$$

where \mathbb{P}_{st} is the diagonal matrix with entries the stalling steady state. **Theorem:** $\tilde{\mathbb{W}}$ is a Markov generator. **Proof:** It follows trivially from the fact that all off-diagonal entries are positive (since all entries of \mathbb{W}_{st} are at most as big as the entries of \mathbb{W}) and that all columns add up to zero \square . A crucial nontrivial feature of the hidden TR dynamics is that exit rates (diagonal elements of $\tilde{\mathbb{W}}$) are the same as for the original dynamics. Furthermore, with respect to the original dynamics \mathbb{W} , the upper-left 2×2 block (the only non-null block of $\mathbb{W} - \mathbb{W}_{\text{st}}$) is unchanged while the rest of the generator undergoes time-reversal with respect to its own stalling steady state. So, in a way, the hidden dynamics is the best attempt to invert all of the steady-state average currents but the observed ones:



However, the inversion of steady currents cannot be exact, because edge-wise current inversion in a subgraph would break Kirchhoff’s law of current conservation at the sites. At a stalling steady state one has $\tilde{\mathbb{W}}(x^{\text{st}}) = \mathbb{W}^\dagger(x^{\text{st}})$, which we call *marginal detailed balance*.

Finally, we are in the position to provide the foundational brick of our construction. **Theorem:** The marginal FR Eq. (14) holds. **Proof:** Associated to any generator is a p.d.f. $P(\mathbf{t})$ over trajectories \mathbf{t} , i.e. single realizations of a continuous-time Markov jump process $\mathbf{t} = (i_1, t_1) \rightarrow (i_2, t_2) \rightarrow \dots \rightarrow (i_N, t_N)$, depicted by a successions of sites and of waiting times before a transition to a new site occurs, up to time $1 = \sum_{n=1}^N t_n$. To dispense with boundary terms, irrelevant at long-enough

time, we assume that the trajectory is cyclic $i_N \equiv i_0$. The trajectory's p.d.f., given the initial site, is a sequence of exponentially distributed waiting times and of instantaneous jump rates (see [21] for a review)

$$P(\mathbf{t}) = e^{-w_{i_N} t_N} \prod_{n=0}^{N-1} w_{i_{n+1}, i_n} e^{-w_{i_n} t_n}. \quad (19)$$

Similarly, we can compute $\tilde{P}(\mathbf{t})$. Same exit rates imply same waiting-time terms in these expressions, yielding:

$$\frac{P(\mathbf{t})}{\tilde{P}(\mathbf{t})} = \prod_{n=0}^{N-1} \frac{w_{i_{n+1}, i_n}}{\tilde{w}_{i_{n+1}, i_n}} = \prod_{ij \neq 12, 21} \left(\frac{w_{ij} p_j^{\text{st}}}{w_{ji} p_i^{\text{st}}} \right)^{J_{ij}^t/2} \quad (20)$$

where the currents are the random variables

$$J_{ij}^t = \sum_{n=0}^{N-1} (\delta_{i, i_{n+1}} \delta_{j, i_n} - \delta_{j, i_{n+1}} \delta_{i, i_n}) \quad (21)$$

counting the net number of transitions ij . Notice that in Eq. (20) we used the fact that hidden TR and original dynamics have the same rates along edge 12. We can now multiply by $1 = e^{-\tilde{F} J^t} (w_{12} p_2^{\text{st}} / w_{21} p_1^{\text{st}})^{J^t}$ to obtain

$$\frac{P(\mathbf{t})}{\tilde{P}(\mathbf{t})} = e^{-\tilde{F} J^t} \prod_{ij} \left(\frac{w_{ij}}{w_{ji}} \right)^{J_{ij}^t} = e^{-\tilde{F} J^t} \frac{P(\mathbf{t})}{\tilde{P}(\mathbf{t})}. \quad (22)$$

In the first passage, the contributions $p_{i_n}^{\text{st}}/p_{i_{n+1}}^{\text{st}}$ cancel out because the trajectory is continuous and cyclic. Finally, in the last passage we used the complete FR, that relates the original and TR probabilities of paths. The theorem then follows by rearranging things around and by marginalizing for the current J^t \square .

Another, more elegant way to derive the result is via the Generating Function of the (time-)Scaled current's Cumulants (SCGF) $\lambda(q) = \langle J^t \rangle q + \frac{1}{2} \text{var}(J^t) q^2 + \dots$. To discuss possible generalizations, we allow for a current supported on several edges, $J^t = \sum_{ij} \varphi_{ij} J_{ij}^t$, with $\varphi_{ij} = -\varphi_{ji}$. The following symmetry coincides with the marginal FT Eq. (14) after a Laplace transform. **Theorem:** *There exists an effective affinity \tilde{F} such that marginal Lebowitz-Spohn symmetry [22] holds*

$$\tilde{\lambda}(q) = \lambda(\tilde{F} - q). \quad (23)$$

Proof: The SCGF can be obtained as the dominant Perron-Frobenius eigenvalue of the so-called *tilted operator* $\mathbb{M}(q)$, which is obtained by replacing off-diagonal entries of the generator by $w_{ij} e^{-\varphi_{ij} q}$, while keeping the diagonal exit rates, e.g. in our single-edge case

$$\mathbb{M}(q) = \begin{pmatrix} -w_1 & w_{12} e^{-q} & w_{13} & w_{14} \\ w_{21} e^q & -w_2 & w_{32} & 0 \\ w_{13} & w_{32} & -w_3 & w_{34} \\ w_{41} & 0 & w_{43} & -w_4 \end{pmatrix}. \quad (24)$$

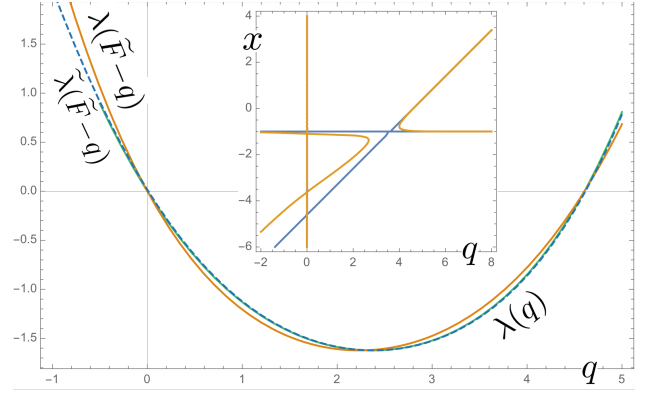


FIG. 1: We consider the model in Eq. (7) with rates $1 = w_{31} = w_{14} = w_{32} = w_{43} = w_{21}/(1+x)$ and $10 = w_{13} = w_{41} = w_{23} = w_{34} e^{-y} = w_{12} e^{-x}/(1+x)$. **Main frame:** For $x = y = 0$, we plot the SCGF $\lambda(q)$ and its symmetric $\lambda(\tilde{F} - q)$; the two do not coincide and only meet at 0 , $\tilde{F}/2$ and \tilde{F} , showing that the FR does not hold. We also plot (dashed) $\tilde{\lambda}(\tilde{F} - q)$, which perfectly coincides with $\lambda(q)$, showing that the FR is restored by the hidden-TR dynamics. **Incept:** When only transition 12 is counted, for $y = 0$, straight lines are the *loci* where $\lambda(q, x) \equiv 0$; apart from the trivial $q = 0$ and $x = -1$ lines, the diagonal line corresponds to the effective affinity $\tilde{F}(x)$, showing that it is linear in x . The curvy lines are obtained when we also count 34 (by setting $\varphi_{ij} = \delta_{i,1}\delta_{j,2} + \delta_{i,3}\delta_{j,4} - (i \leftrightarrow j)$ and $y = x$). The effective affinity is no longer linear in x .

The SCGF always vanishes at $q = 0$. Since it's convex, unless it does not have a finite minimum (which might be the case in certain interacting particle models displaying phase transitions) there will exist another value $q = \tilde{F}$ at which $\lambda(\tilde{F}) = 0$. One can then build a new Markov generator by Doob's transform $\tilde{\mathbb{W}} = \mathbb{L}^{-1} \mathbb{M}(\tilde{F})^T \mathbb{L}$, where \mathbb{L} is the diagonal matrix containing the entries of the left-null eigenvector of $\mathbb{M}(\tilde{F})$. In the single-edge case, direct computation returns Eq. (17). We can furthermore obtain the SCGF $\tilde{\lambda}(q)$ of the hidden dynamics as the dominant eigenvalue of the tilted operator $\tilde{\mathbb{M}}(q) = \mathbb{L}^{-1} \mathbb{M}(\tilde{F} - q)^T \mathbb{L}$, which is a similarity of matrices \square .

In Fig. 1 the plot of the SCGF for the original and the hidden TR dynamics, and their symmetric obtained by $q \rightarrow \tilde{F} - q$, clearly shows that the marginal FR holds. The latest derivation seems to imply that our results generalize to the situation where several transitions contribute to the observable current; *mathematically*, all is needed is that there exists another value $q = \tilde{F}$ at which $\lambda(\tilde{F}) = 0$. However, in our previous *physical* construction it was crucial that the effective affinity was linear in the thermodynamic parameter x (see [24]), and that $\mathbb{L} = \mathbb{P}_{\text{st}}^{-1}$ could be interpreted as the stalling steady-state. This is not the case in general, as shown in the incept in Fig. 1. Hence one must be prudent in claiming generality. A thorough discussion of the complex case of multiple currents supported on several edges [23] is in preparation.

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- [24] Notice that all such affinities are either in the form $F_\alpha(x) = x - x_\alpha^*$ or do not depend on x . Therefore the explicit derivative with respect to x is akin to the implicit variation of the affinities ∂_{F_α} or, equivalently, $\partial_{\bar{F}}$, which are usually encountered in response theory.